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SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Stu Hendryson Examiner #: 66652 Date: 11/30
 Art Unit: 1754 Phone Number 303-2539 Serial Number: 51818
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If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: C36

Inventors (please provide full names): Piskoti, Zoltan, Marvin Cohen

Earliest Priority Filing Date: 3/99

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

C36 fullerenes/fullerite.

36 carbon atom cluster

Please do not flood me with C60, C70, C84 stuff!

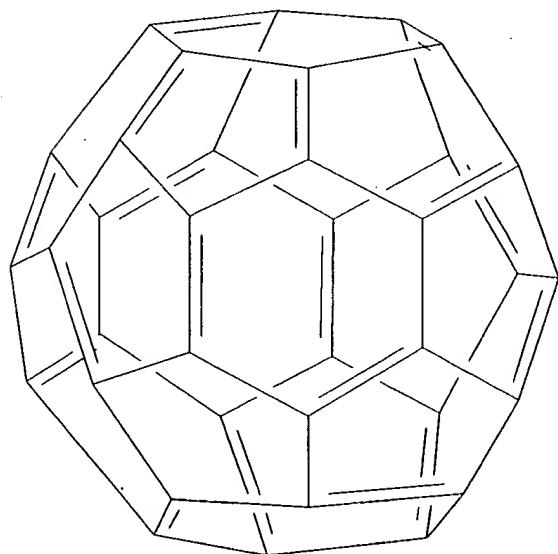
STAFF USE ONLY		Type of Search	Vendors and cost where applicable
Searcher: <u>EJ</u>		NA Sequence (#) _____	STN <u>168-10</u>
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Clerical Prep Time: _____		Patent Family _____	WWW/Internet _____
Online Time: <u>145</u>		Other _____	Other (specify) _____

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L11 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2001 ACS
 RN 144161-03-5 REGISTRY
 CN [5,6]Fullerene-C36-D6h (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN Fullerene-C36-D6h
 MF C36
 CI COM, RPS
 SR CA
 LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C5-C5-C5-C5-	C5-C5-C5-C5-	5-5-5-5-5-5-	C36	53661.1.1	1
C5-C5-C5-C5-	C5-C5-C5-C5-	5-5-5-5-5-5-			
C5-C5-C5-C5-	C5-C5-C5-C5-	6-6-6-6-6-6-			
C6-C6-C6-C6-	C6-C6-C6-C6-	6			
C6-C6-C6	C6-C6-C6				



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 2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

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DICTIONARY FILE UPDATES: 30 JUL 2001 HIGHEST RN 349531-86-8

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DEL HIS Y

E C36/MF

L1 47 S E3

L2 12383 S FULLERENE#

L3 35 S L1 AND L2

FILE 'HCAPLUS' ENTERED AT 15:12:38 ON 31 JUL 2001

L4 19 S PISKOTI ?/AU

L5 355 S ZETTL ?/AU

L6 28891 S COHEN ?/AU

L7 2006 S COTE ?/AU

L8 3574 S GROSSMAN ?/AU

L9 959 S LOUIE ?/AU

L10 1 S L4 AND L5 AND L6 AND L7 AND L8 AND L9
SEL

L10 1 RN

FILE 'REGISTRY' ENTERED AT 15:14:12 ON 31 JUL 2001

L11 1 S E1

FILE 'CAOLD' ENTERED AT 15:14:18 ON 31 JUL 2001

L12 0 S L11

FILE 'HCAPLUS' ENTERED AT 15:14:24 ON 31 JUL 2001

L13 61 S L11

FILE 'STNGUIDE' ENTERED AT 15:15:21 ON 31 JUL 2001

L14 FILE 'HCAPLUS' ENTERED AT 15:20:02 ON 31 JUL 2001
1066392 S SPECTRO?

L15 15804 S SCAN?(3A) TUNNEL?

FILE 'LCA' ENTERED AT 15:20:04 ON 31 JUL 2001
L16 2475 S 76/SC, SX
L17 3233 S 73/SC, SX

FILE 'REGISTRY' ENTERED AT 15:20:27 ON 31 JUL 2001

FILE 'HCAPLUS' ENTERED AT 15:22:28 ON 31 JUL 2001
L18 3 S L13 AND L14
L19 1 S L13 AND L15
L20 5 S L13 AND L16
L21 8 S L13 AND L17
L22 0 S L20 AND L21
L23 25 S L13 AND 1967-1998/PY
L24 13 S L18 OR L19 OR L20 OR L21
L25 8 S L24 AND 1967-1999/PY
L26 7 S L25 NOT L10
L27 21 S L23 NOT L26
L28 25 S L13 AND 1967-1998/PY
L29 0 S L28 NOT (L26 OR L27)
L30 39 S L13 AND 1967-1999/PY
L31 11 S L30 NOT (L26 OR L27)

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FILE 'HCAPLUS' ENTERED AT 15:34:33 ON 31 JUL 2001

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FILE LAST UPDATED: 30 Jul 2001 (20010730/ED)

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=> d 126 1-7 ibib abs hitind

L26 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1999:758983 HCAPLUS
DOCUMENT NUMBER: 132:142218
TITLE: Vibronic interactions in the C36 tri- and tetra-anions
AUTHOR(S): Yoshizawa, Kazunari; Tachibana, Masamitsu; Yamabe, Tokio
CORPORATE SOURCE: Department of Molecular Engineering, Kyoto University, Sakyo-ku, Kyoto, 606-8501, Japan
SOURCE: J. Chem. Phys. (1999), 111(22), 10088-10092
CODEN: JCPSA6; ISSN: 0021-9606
PUBLISHER: American Institute of Physics
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We address the intramol. vibronic interactions in the C36 tri- and tetra-anions to understand the Jahn-Teller effects and possible supercond. in "electron-doped" C36 solids. We use the B3LYP hybrid Hartree-Fock/d.-functional-theory method for our theor. analyses. Neither the HOMO (HOMO) nor the LUMO (LUMO) of the C36 mol. with D6h symmetry are degenerate, but the next LUMO is twofold degenerate. One can therefore expect Jahn-Teller distortions and interesting electronic properties in the C36 anions. Computed vibronic and electron-phonon coupling consts. of the tetra-anion are about twice as large as those of the tri-anion. The second lowest Jahn-Teller active E2g mode of 561 cm-1 is predicted to have the largest coupling consts. in both anions. We calc. superconducting transition temp. Tc from McMillan's formula using the coupling consts. as well as electronic densities of states at the Fermi level and Coulomb pseudopotentials as parameters.

CC 65-5 (General Physical Chemistry)
Section cross-reference(s): 76
IT 144161-03-5, Fullerene C36 d6h 256482-38-9,
[5,6]Fulleride(3-) -C36-D6h 256482-39-0, [5,6]Fulleride(4-) -C36-D6h
(vibronic interactions in C36 tri- and tetra-anions)

REFERENCE COUNT: 29
REFERENCE(S):
(1) Asai, Y; Phys Rev B 1992, V46, P1265 HCAPLUS
(2) Becke, A; J Chem Phys 1993, V98, P5648
HCAPLUS
(3) Becke, A; Phys Rev A 1988, V38, P3098
HCAPLUS
(6) Ceulemans, A; Structure and Bonding 1989,

V71 HCAPLUS

(7) Conwell, E; Phys Rev B 1980, V22, P1761
HCAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2001 ACS
 ACCESSION NUMBER: 1999:489905 HCAPLUS
 DOCUMENT NUMBER: 131:219384
 TITLE: Electronic and structural properties of C36 molecule
 AUTHOR(S): Yu, Xiaoqing; Wu, Congjun; Wang, Chui-Lin; Su, Zhao-Bin
 CORPORATE SOURCE: Department of Physics, Peking University, Beijing, 100871, Peop. Rep. China
 SOURCE: Int. J. Mod. Phys. B (1999), 13(12), 1513-1523
 CODEN: IJPBEV; ISSN: 0217-9792
 PUBLISHER: World Scientific Publishing Co. Pte. Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The extended SSH model and Bogolyubov-de-Gennes (BdeG) formalism are applied to investigate the electronic properties and stable lattice configurations of C36. We focus the problem on the mol.'s unusual D6h symmetry. The electronic part of Hamiltonian without Coulomb interaction is solved anal. We found that the gap between HOMO and LUMO is small due to the long distance hopping between the 2nd and 5th layers. The charge densities of HOMO and LUMO states are mainly distributed in the two layers, that causes a large splitting between the spin triplet and singlet excitons. The differences of bond lengths, angles and charge densities among mol. and polarons are discussed.

CC 65-5 (General Physical Chemistry)
 Section cross-reference(s): 73, 77

IT 144161-03-5, [5,6]Fullerene-C36-D6h
 (electronic and structural properties of C36 mol. studied theor.)

REFERENCE COUNT: 8
 REFERENCE(S):
 (1) Cote, M; Phy Rev Lett 1998, V81, P697
 HCAPLUS
 (2) Deng, Y; Phys Lett 1992, VA170, P116
 (3) Grossman, J; Chem Phys Lett 1998, V284, P344
 HCAPLUS
 (4) Heath, J; Nature 1998, V393, P730 HCAPLUS
 (5) Piskoti, C; Nature 1998, V393, P771 HCAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2001 ACS
 ACCESSION NUMBER: 1999:87156 HCAPLUS
 DOCUMENT NUMBER: 130:242505
 TITLE: Resonance stabilization study of some fullerenes C_n(20 .ltoreq. n .ltoreq. 88): is n = 32 a 'magic' number?
 AUTHOR(S): Zahedi, Mansour; Latif, Mohammed Al-Kobaisi

CORPORATE SOURCE: Faculty of Sciences, Department of Chemistry,
 Shahid Beheshti University, Tehran, Iran
 SOURCE: J. Chem. Res., Synop. (1999), (1),
 52-53
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A .pi.-orbital axis vector (POAV) anal. used in HMO approxn. calcns.
 indicates that the cutoff in the fullerene mass spectrum at C_n (n =
 32) must naturally occur with no need to define a 'magic' no.
 CC 65-5 (General Physical Chemistry)
 Section cross-reference(s): 73
 IT 99685-96-8, [5,6]Fullerene-C60-Ih 104375-45-3, [5]Fullerene-C20-Ih
 115383-19-2, [5,6]Fullerene-C28-Td 115383-20-5,
 [5,6]Fullerene-C32-D3 115383-21-6, [5,6]Fullerene-C50-D5h(6)
 115383-22-7, [5,6]Fullerene-C70-D5h(6) 133947-14-5,
 [5,6]Fullerene-C80-Ih 135026-72-1, [5,6]Fullerene-C30-D5h
 139707-95-2, [5,6]Fullerene-C78-D3 142870-58-4,
 [5,6]Fullerene-C24-D6d 142870-59-5, [5,6]Fullerene-C26-D3h
 144161-03-5, [5,6]Fullerene-C36-D6h 145646-79-3,
 [5,6]Fullerene-C42-D3 146269-86-5, [5,6]Fullerene-C40-Td
 146401-64-1, [5,6]Fullerene-C38-C3v 147230-75-9,
 [5,6]Fullerene-C80-D2 153843-94-8, [5,6]Fullerene-C34-C3v
 153843-96-0, [5,6]Fullerene-C48-D3
 (resonance stabilization study of some fullerenes C_n (20 .ltoreq.
 n .ltoreq. 88): is n = 32 a 'magic' no.)
 REFERENCE COUNT: 15
 REFERENCE(S):
 (1) Balasubramanian, K; J Phys Chem 1995, V99,
 P6509 HCPLUS
 (2) Ballone, P; Phys Rev B 1990, V42, P3201
 HCPLUS
 (3) Curl, R; Science 1988, V242, P1017 HCPLUS
 (5) Dietz, T; J Chem Phys 1981, V74, P6511
 HCPLUS
 (6) Eggen, B; J Chem Soc Faraday Trans 1994,
 V90, P3029 HCPLUS
 ALL CITATIONS AVAILABLE IN THE RE FORMAT
 L26 ANSWER 4 OF 7 HCPLUS COPYRIGHT 2001 ACS
 ACCESSION NUMBER: 1998:727819 HCPLUS
 DOCUMENT NUMBER: 130:115319
 TITLE: § Polyhedral carbon clusters C_{36+12n} (n .gtoreq.
 0) and their hydrocarbon analogs as predecessors
 of (6,0)-tubular structures
 Stankevich, I. V.; Chistyakov, A. L.; Gal'pern,
 E. G.; Chernozatonskii, L. A.
 Institute of Organoelement Compounds of RAS,
 Moscow, 117813, Russia
 AUTHOR(S):
 CORPORATE SOURCE: Mol. Cryst. Liq. Cryst. Sci. Technol., Sect. C (1998), 10(1-4), 169-174
 SOURCE: CODEN: MOMAEAO; ISSN: 1058-7276

PUBLISHER: Gordon & Breach Science Publishers
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Mol. and electronic structure of prolate-shape carbon clusters C_{36+12n} (n > 0) were studied by topol. and valence approaches. Asymptotic properties of the cluster spectra are discussed. Structures of some polyhedral hydrocarbons being predecessors of (6,0)-tubular structures are also calcd. by the MNDO/PM3 method.
 CC 65-5 (General Physical Chemistry)
 Section cross-reference(s): 73
 IT 144161-03-5, [5,6]Fullerene-C36-D6h 170032-24-3,
 [5,6]Fullerene-C60-D6h 175698-20-1, [5,6]Fullerene-C48-D6d(5)
 218957-99-4 218958-05-5 218959-88-7, [5,6]Fulleride(2-) -C36-D6h
 218959-93-4, [5,6]Fulleride(2-) -C48-D6d(5) 218960-00-0,
 [5,6]Fulleride(2-) -C60-D6h 218960-22-6 218960-23-7
 219606-80-1, [5,6]Fullerene-C72-D6d(5) 219607-06-4,
 [5,6]Fulleride(2-) -C72-D6d(5)
 (MNDO-PM3 study of polyhedral carbon clusters C_{36+12n} (n > 0) and hydrocarbon analogs as predecessors of tubular structures)
 REFERENCE COUNT: 4
 REFERENCE(S):
 (1) Kratschmer, W; Nature 1990, V347, P354
 (2) Kroto, H; Nature 1985, V318, P162 HCPLUS
 (3) Sokolov, V; Usp Khim 1993, V62, P455 HCPLUS
 (4) Stankevich, I; Mol Mater 1996, V7, P1
 HCPLUS

L26 ANSWER 5 OF 7 HCPLUS COPYRIGHT 2001 ACS
 ACCESSION NUMBER: 1998:638727 HCPLUS
 DOCUMENT NUMBER: 129:306708
 TITLE: Electronic, structural and superconducting properties of molecular and solid C₃₆
 Cote, Michel; Grossman, Jeffrey C.; Cohen, Marvin L.; Louie, Steven G.
 AUTHOR(S):
 CORPORATE SOURCE: Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720, USA
 SOURCE: Proc. - Electrochem. Soc. (1998), 98-8(Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials), 33-46
 CODEN: PESODO; ISSN: 0161-6374

PUBLISHER: Electrochemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Among the exptl. obsd. structures of mol. C₃₆, our calcns. show that the structure with D_{6h} symmetry is one of the most energetically favorable. Based on these results and the fact that D_{6h} is conducive to forming a periodic system, we propose a new solid phase of carbon using C₃₆ fullerenes as a basis. Full structural relaxations are performed and electronic d. of states are evaluated

using an ab initio pseudopotential plane wave method within the local d. approxn. The calcd. electron-phonon interaction potential is found to be substantially enhanced compared to C₆₀, leading to the possibility of larger superconducting transition temps. than in alkali-doped C₆₀ solids.

CC 65-3 (General Physical Chemistry)
 Section cross-reference(s): 75, 76
 IT 144161-03-5, [5,6] Fullerene-C₃₆-D_{6h} 144636-60-2,
 properties
 (electronic, structural, and superconducting properties of mol.
 and solid C₃₆ studied theor.)

L26 ANSWER 6 OF 7 HCPLUS COPYRIGHT 2001 ACS
 ACCESSION NUMBER: 1998:473796 HCPLUS
 DOCUMENT NUMBER: 129:224088
 TITLE: Electron-Phonon Interactions in Solid C₃₆
 AUTHOR(S): Cote, Michel; Grossman, Jeffrey C.; Cohen, Marvin L.; Louie, Steven G.
 CORPORATE SOURCE: Berkeley and Materials Sciences Division,
 Department of Physics, Lawrence Berkeley National Laboratory, University of California,
 Berkeley, CA, 94720, USA
 SOURCE: Phys. Rev. Lett. (1998), 81(3), 697-700
 CODEN: PRLTAO; ISSN: 0031-9007
 PUBLISHER: American Physical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Among the exptl. obsd. structures of mol. C₃₆, the authors' calcns. show that the structure with D_{6h} symmetry is one of the two most energetically favorable. Based on this result and the fact that D_{6h} is conducive to forming a periodic system, the authors propose a new solid phase of C using C₃₆ fullerenes as a basis. Full structural relaxations and electronic d. of states are evaluated using an ab initio pseudopotential plane wave method within the local d. approxn. The calcd. electron-phonon interaction potential is substantially enhanced compared to C₆₀, leading to the possibility of larger superconducting transition temps. than in alkali-doped C₆₀ solids.

CC 76-4 (Electric Phenomena)
 IT 144161-03-5, [5,6] Fullerene-C₃₆-D_{6h}
 (supercond. in C₃₆ fullerene)

L26 ANSWER 7 OF 7 HCPLUS COPYRIGHT 2001 ACS
 ACCESSION NUMBER: 1998:438859 HCPLUS
 DOCUMENT NUMBER: 129:144128
 TITLE: C₃₆, a new carbon solid
 AUTHOR(S): Piskoti, C.; Yarger, J.; Zettl, A.
 CORPORATE SOURCE: Dep. of Phys., Univ. of California, Berkeley,
 CA, 94720, USA
 SOURCE: Nature (London) (1998), 393(6687), 771-774

CODEN: NATUAS; ISSN: 0028-0836

PUBLISHER: Macmillan Magazines
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Low-mass fullerenes are of particular interest because their high curvature and increased strain energy owing to adjacent pentagonal rings could lead to solids with unusual intermol. bonding and electronic properties. Here the authors report the synthesis of the solid form of C36 by the arc-discharge method. The authors have developed purifn. methods that sep. C36 from amorphous carbon and other fullerenes, to yield satd. solns., thin films and polycryst. powders of the pure solid form. Solid-state NMR measurements suggest that the mol. has D6h sym., and electron-diffraction patterns are consistent with a tightly bound mol. solid with an intermol. spacing of 6.68 .ANG.. The authors observe large increases in the elec. cond. of the solid on doping with alkali metals.

CC 78-1 (Inorganic Chemicals and Reactions).

Section cross-reference(s): 76

IT 144161-03-5P, Fullerene-C36-D6h
 (prepn., ^{13}C NMR, elec. cond., electron diffraction and intercalation with sodium and potassium)

=> d 127 1-21 cbib abs hitrn

L27 ANSWER 1 OF 21 HCPLUS COPYRIGHT 2001 ACS

1998:638726 Document No. 129:321523 Computing temperature-dependent relative stabilities of isomeric fullerenes and quasi-fullerenes. Slanina, Zdenek; Zhao, Xiang; Osawa, Eiji (Laboratories of Computational Chemistry & Fullerene Science, Department of Knowledge-Based Information Engineering, Toyohashi University of Technology, Aichi, 441-8580, Japan). Proc. - Electrochem. Soc., 98-8 (Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials), 21-32 (English) 1998. CODEN: PESODO.

ISSN: 0161-6374. Publisher: Electrochemical Society.

AB Three systems of isomeric fullerenes are computed at semiempirical and ab initio quantum-chem. levels: C94, C36, and C72. The complete set of 134 isolated-pentagon-rule (IPR) isomers of C94 is described by the SAM1 quantum-chem. method, and their energetics is also checked by ab initio SCF computations (HF/3-21G, HF/4-31G), and by the MNDO, AM1, and PM3 semiempirical methods. All the methods point out a C2 species as the system ground state. C36 is also primarily computed at the SAM1 level, and partially also at the HF/4-31G and B3LYP/6-31G* levels. Altogether 598 cages are generated by a topol. Stone-Wales treatment. Three cages turn out to be particularly important, two conventional fullerenes with D2d and C2v symmetries and a C5 quasi-fullerene contg. one four-membered ring. Finally, the SAM1 method is applied to C72, both the solitary IPR structure and several non-IPR isomers. For all three isomeric systems, the computed energetics is combined with calcd. entropy contributions so

that a proper Gibbs free energy treatment is possible. Considerable temp. effects on the isomeric relative stabilities are reported, having a substantial impact on the theory-expt. comparisons.

IT 144161-03-5, [5,6] Fullerene-C36-D6h

(computing temp.-dependent relative stabilities of isomeric fullerenes and quasi-fullerenes)

L27 ANSWER 2 OF 21 HCAPLUS COPYRIGHT 2001 ACS

1998:171706 Document No. 128:326760 Electronic and structural properties of molecular C36. Grossman, Jeffrey C.; Cote, Michel; Louie, Steven G.; Cohen, Marvin L. (University of California at Berkeley and Materials Sciences Division, Department of Physics, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720, USA). Chem. Phys. Lett., 284(5,6), 344-349 (English) 1998.

CODEN: CHPLBC. ISSN: 0009-2614. Publisher: Elsevier Science B.V..

AB Electronic and structural properties of several isomers of mol. C36 are investigated using the pseudopotential d. functional approach. These calcns. show that substitutional doping with nitrogen can lead to a 10% decrease in the C-C bond lengths of C36, and this effect is explained using a simple example. Further, we have calcd. endohedral binding energies and demonstrate that C36 is perhaps the smallest fullerene size which can easily trap a range of atoms. The NMR chem. shifts, evaluated for the two lowest energy fullerene isomers, show that they are sufficiently different chem. to be distinguishable exptl.

IT 144161-03-5, [5,6] Fullerene-C36-D6h

(electronic and structural properties of isomers of mol. C36)

L27 ANSWER 3 OF 21 HCAPLUS COPYRIGHT 2001 ACS

1998:20125 Document No. 128:159120 Correlation between energies of proper fullerenes and their topological invariants. Part I. Fullerenes with abutting pentagons. Balaban, Alexandru T.; Ivanciu, Ovidiu; Babic, Darko (Department of Organic Chemistry, University "Politehnica" of Bucharest, Bucharest, 78100, Rom.). Fullerene Sci. Technol., 5(7), 1479-1506 (English) 1997.

CODEN: FTECEG. ISSN: 1064-122X. Publisher: Marcel Dekker, Inc..

AB For all constitutional isomers of proper fullerenes with N = 50 and 60 carbon atoms, correlations for mol. mechanics-derived energies with r around 0.98 were developed by multi-linear regression using four to six mol. descriptors. The descriptors are based on the sizes and disposition of polygons surrounding each edge. By treating sep. the 1812 C60 isomers and the 271 C50 isomers, std. deviations around 4.2 and 3.3 kcal/mol, resp., were obtained; if one combines all these isomers and if one includes the no. of carbon atoms as an addnl. descriptor, std. deviations s of about 4.0 kcal/mol result. For systems with N < 50 carbon atoms, the correlations are less good.

IT 144161-03-5, Fullerene (C36)-D6h

(correlation between energies of proper fullerene isomers and topol. invariants: fullerenes with abutting pentagons)

L27 ANSWER 4 OF 21 HCAPLUS COPYRIGHT 2001 ACS

1997:753556 Document No. 128:93388 Optimization of carbon cluster geometry using a genetic algorithm. Hobday, Steven; Smith, Roger (Department of Mathematical Sciences, Loughborough University, Leicestershire, LE11 3TU, UK). J. Chem. Soc., Faraday Trans., 93(22), 3919-3926 (English) 1997. CODEN: JCFTEV. ISSN: 0956-5000. Publisher: Royal Society of Chemistry.

AB A genetic algorithm (GA) based global optimization procedure has been developed and used to find the most stable configurations of small carbon clusters. The GA attempts to locate the set of at. nuclei coordinates assocd. with the global min. of the potential-energy function using an analogy to Darwinian natural selection. This algorithm uses a novel encoding scheme to evolve a population of cluster geometries towards a low-energy final state. Two semi-empirical many-body potential-energy functions have been encoded for carbon interactions. The binding energies and structural forms of carbon clusters between C3 and C60 are reported. It has been shown that the algorithm can det. structures with a lower energy than those previously published using more classical local optimization procedures. The GA can also be used to predict the global minimal energy configuration of pairwise interaction potentials.

IT 144161-03-5, Fullerene-C36-D6h
(optimization of carbon cluster geometry using genetic algorithm)

L27 ANSWER 5 OF 21 HCAPLUS COPYRIGHT 2001 ACS

1997:388857 Document No. 127:140921 Permanents of adjacency matrixes of fullerenes. Cash, Gordon G. (Health Environmental Review Division, U.S. Environmental Protection Agency, Washington, DC, 20460, USA). Polycyclic Aromat. Compd., 12(1), 61-69 (English) 1997. CODEN: PARCEO. ISSN: 1040-6638. Publisher: Gordon & Breach.

AB This study examines the relationships between structural parameters for 28 fullerenes and the permanents of their adjacency matrixes, per(A). In particular, the structural parameters examd. were related to the adjoining of pentagons. A new parameter, r, was introduced which counts contiguous pentagon triplets that have no single vertex in common. The quantity well-correlated with structure was not per(A) itself, but $\ln[\text{per}(A)]/\ln K$, where K is the Kekule structure count. For all 28 fullerenes, $\ln[\text{per}(A)]/\ln K > 2$, contrary to expectations.

IT 144161-03-5, [5,6]Fullerene-C36-D6h
(permanents of adjacency matrixes of fullerenes)

L27 ANSWER 6 OF 21 HCAPLUS COPYRIGHT 2001 ACS

1996:393608 Document No. 125:42275 Determination of Topological Equivalence Classes of Atoms and Bonds in C20-C60 Fullerenes Using a New Prolog Coding Program. Laidboeur, Thierry; Cabrol-Bass, Daniel; Ivanciu, Ovidiu (LARTIC, University of Nice-Sophia Antipolis, Nice, 06108, Fr.). J. Chem. Inf. Comput. Sci., 36(4), 811-821 (English) 1996. CODEN: JCISD8. ISSN: 0095-2338.

AB A new general mol. coding Prolog program is used in theor. studies of the properties of fullerene isomers and derivs. to identify the

topol. equivalence classes of atoms and bonds in C₂₀-C₆₀ fullerenes. The symmetry perception algorithm is based on an exhaustive search of a minimal code. During this search all canonical labeled mapping trees are generated, allowing construction of equivalence classes of atoms and bonds. Although the present algorithm makes a complete search of canonical labelings in the mol. graph, computational time is kept within reasonable limits even for large regular graphs such as fullerenes. In the case of fullerenes, topol. equivalence classes of atoms allow easy generation of heterofullerene isomers, while the bond classes allow for the generation of addn. or cycloaddn. isomers. The no. of atom classes and the no. of atoms in each class give important information on the no. of ¹³C NMR signals and intensity patterns in fullerenes.

IT 144161-03-5, [5,6]Fullerene-C36-D6h
(topol. equivalence classes of atoms and bonds in C₂₀-C₆₀ fullerenes using a Prolog coding program)

L27 ANSWER 7 OF 21 HCAPLUS COPYRIGHT 2001 ACS
1996:187036 Document No. 124:299345 Local softness and hardness as reactivity indices in the fullerenes C₂₄-C₇₆. Choho, K.; Langenaeker, W.; Van de Woude, G.; Geerlings, P. (Eenheid Algemene chemie (ALGC), Faculteit Wetenschappen, Vrije Universiteit Brussel, Pleinlaan 2, Brussels, 1050, Belg.). THEOCHEM, 362(3), 305-15 (English) 1996. CODEN: THEODJ. ISSN: 0166-1280.

AB The condensed local softness, sk+ or condensed Fukui function, fk+, approximated by Mulliken at. charge differences, are used as a descriptor of the regioselectivity for the fullerenes (from C₂₄ to C₇₆) towards a nucleophilic attack. In general the results, which are in agreement with exptl. data, can be interpreted in terms of a pyramidalization angle effect, soft-hard alternations and softness delocalization. The local hardness on the most reactive carbon atom in each fullerene turns out to be a valuable descriptor of the intermol. reactivity sequence. The maximal hardness principle is used to discuss the stability for the larger fullerenes (C₅₀, C₆₀, C₇₀ and C₇₆). The calcd. hardness, approx. calcd. as the LUMO-HOMO energy difference, confirms the fact that C₆₀ and C₇₀ are the most stable fullerenes.

IT 144161-03-5, [5,6]Fullerene-C36-D6h
(local softness and hardness as reactivity indexes in fullerenes C₂₄-C₇₆ studied theor.)

L27 ANSWER 8 OF 21 HCAPLUS COPYRIGHT 2001 ACS
1996:173153 Document No. 124:299339 Electronic structures of dihedral (D_{5h}, D_{5d}, D_{6h}, D_{6d}) fullerenes. Tang, Au Chin; Huang, Fu Qiang (Institute of Theoretical Chemistry, Jilin University, Changchun, 130023, Peop. Rep. China). Chem. Phys. Lett., 250(5,6), 528-36 (English) 1996. CODEN: CHPLBC. ISSN: 0009-2614.

AB By means of our proposed method for Hueckel theory calcn., we have calcd. the electronic structures of dihedral (D_{5h}, D_{5d}, D_{6h}, D_{6d}) fullerenes, which are generated from icosahedral C₂₀, C₆₀, C₈₀, C₁₈₀, C₂₄₀ and C₅₄₀, resp. From the calcd. results of 1224 fullerene mols., certain rules on the stability and chem. reactivity

IT have been drawn for such types of dihedral fullerenes.
144161-03-5, [5,6]Fullerene-C36-D6h
 (electronic structures of dihedral (D5h, D5d, D6h, D6d) fullerenes)

L27 ANSWER 9 OF 21 HCPLUS COPYRIGHT 2001 ACS
 1995:1005199 Document No. 124:156512 A MNDO study of carbon clusters with specifically fitted parameters. Tseng, Shiuh-ping; Shen, Min-yi; Yu, Chin-hui (Dep. Chem., National Tsing Hua Univ., Hsinchu, 300, Taiwan). Theor. Chim. Acta, 92(5), 269-80 (English) 1995. CODEN: TCHAAM. ISSN: 0040-5744.

AB A MNDO method with new parameters for C clusters is presented. The parameters in the new sets were specifically tuned to fit the properties of small C clusters, C2, C3, C5, and C7-C10, and buckminsterfullerene, C60. The validity of these MNDO parameters was verified by exptl. data. The calcd. (with new parameters) IR spectra of C60 and the heat of formation, geometry, and IR spectra of C70 agree satisfactorily with obsd. data. Heats of formation of other fullerenes, from C20-C84, and C600 are evaluated. The resulting heats of formation of the isomers of C76 and C84 are reliable and their relative stability is in excellent agreement with other reports. The predicted IR spectra of several fullerenes, C24(C6v), C28(Td), C32(D3), C36(D6h), C50(C5h) and C80(D5d) are provided to aid assignments of exptl. spectra.

IT **144161-03-5**, [5,6]Fullerene-C36-D6h
 (MNDO study of carbon clusters with specifically fitted parameters as well as IR spectra and heat of formation calcn.)

L27 ANSWER 10 OF 21 HCPLUS COPYRIGHT 2001 ACS
 1995:765704 Document No. 123:209188 Closed-shell electronic requirements for small fullerene cage structures. Fan, Man-Fai; Lin, Zhenyang; Yang, Shihe (Department of Chemistry, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong). THEOCHEM, 337(3), 231-40 (English) 1995. CODEN: THEODJ. ISSN: 0166-1280.

AB Hueckel model calcns. have been performed for small fullerene cages with 20-50 atoms. The closed-shell electronic structures for the small cages are emphasized. The relatively high stability of C24, C28, C32, C44 and C50 clusters obsd. in the early laser vaporization expts. is explained. These clusters have pseudo closed-shell or half-filled electronic structures with a relatively large HOMO-LUMO gap. Based on the Heuckel results, a large no. of other possible stable clusters is proposed formed by adding hydrogens, replacing carbons with other atoms which have an appropriate no. of valence electrons, or encapsulating metal atoms capable of donating a given no. of valence electrons.

IT **144161-03-5**, Fullerene C36-D6h
 (closed-shell electronic requirements for stability of)

L27 ANSWER 11 OF 21 HCPLUS COPYRIGHT 2001 ACS
 1995:627656 Document No. 123:123649 Distance Spectra and Distance Polynomials of Fullerenes. Balasubramanian, K. (Department of

Chemistry and Biochemistry, Arizona State University, Tempe, AZ, 85287-1604, USA). J. Phys. Chem., 99(27), 10785-96 (English) 1995. CODEN: JPCHAX. ISSN: 0022-3654.

AB Distance matrixes of fullerenes are obtained which contain important topol. information. By use of these matrixes, distance level patterns are constructed which uniquely characterize fullerenes and thus appear to be topol. invariants. The distance spectra and characteristic polynomials of the distance matrixes of C20-C90 fullerenes are computed as well as the Wiener topol. indexes. The sums of powers of the distance spectra are computed and considered as structural invariants.

IT 144161-03-5, [5,6]Fullerene-C36-D6h
(topol., distance spectra and distance polynomials of fullerenes C20-C90)

L27 ANSWER 12 OF 21 HCPLUS COPYRIGHT 2001 ACS
1995:286502 Document No. 122:144042 Theoretical evaluations of standard heats of formation of fullerenes. An accurate semi-empirical method. Tseng, Shiu-h-ping; Yu, Chin-hui (Department of Chemistry, National Tsing Hua University, Hsinchu, 300, Taiwan). Chem. Phys. Lett., 231(4,5,6), 331-6 (English) 1994.

CODEN: CHPLBC. ISSN: 0009-2614.

AB A new set of MNDO parameters is obtained by fitting ref. data from small carbon clusters and exptl. data for C60. This set of parameters was applied to a series of fullerenes, ranging from C20 to C80, and yielded good results for geometries and heats of formation; for example, the estd. heat of formation of C70 is excellent. This set of parameters was also applied to fullerene derivs., giving results in agreement with HF ab initio calcns. MNDO with the new parameters can also be used to evaluate the geometries and IR frequencies of C60 and C70.

IT 144161-03-5, [5,6]Fullerene-C36-D6h
(heat of formation MNDO evaluation for)

L27 ANSWER 13 OF 21 HCPLUS COPYRIGHT 2001 ACS
1995:67211 Document No. 122:17505 Graph-theoretical characterization of fullerene cages. Balasubramanian, K. (Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ, 85287-1604, USA). Polycyclic Aromat. Compd., 3(4), 247-59 (English) 1993. CODEN: PARCEO. ISSN: 1040-6638.

AB Graph-theor. characterizations of fullerene cages C_n [$n = 20-90$] based on the characteristic polynomials of these cages are outlined. It is shown that in general at least the first eleven non-zero coeffs. in the characteristic polynomials are needed to distinguish carbon cages up to C90. No isospectral fullerene cages have been found up to C90.

IT 144161-03-5, [5,6]Fullerene-C36-D6h
(graph-theor. characteristic polynomials of)

L27 ANSWER 14 OF 21 HCPLUS COPYRIGHT 2001 ACS
1994:564353 Document No. 121:164353 Laplacian polynomials of fullerenes (C20-C40). Balasubramanian, K. (Department of Chemistry

and Biochemistry, Arizona State University, Tempe, AZ, 85287-1604, USA). Chem. Phys. Lett., 224(3-4), 325-32 (English) 1994. CODEN: CHPLBC. ISSN: 0009-2614.

AB The characteristic polynomials of the Laplacian matrixes of small fullerenes (C₂₀-C₄₀) are obtained. These polynomials are useful in not only characterizing the structures of fullerenes but also in some of their vibrational modes. The Laplacians of C₂₀, C₂₄, C₂₈, C₃₂, C₃₆, C₃₈ and C₄₀ fullerenes were found to have at least one non-zero integral eigenvalue. The factorization of Laplacian polynomials of some of these fullerenes is also considered.

IT 144161-03-5, [5,6]Fullerene-C36-D6h
(Laplacian polynomials of)

L27 ANSWER 15 OF 21 HCPLUS COPYRIGHT 2001 ACS

1994:331648 Document No. 120:331648 Topological resonance energy predictions of the stability of fullerene clusters. Manoharan, M.; Balakrishnarajan, M. M.; Venuvanalingam, P.; Balasubramanian, K. (Department of Chemistry, Bharathidasan University, Tiruchirarpalli 620024, Tamilnadu, India). Chem. Phys. Lett., 222(1-2), 95-100 (English) 1994. CODEN: CHPLBC. ISSN: 0009-2614.

AB The topol. resonance energies (TRE) for various fullerenes (C₂₀ to C₆₀) were calcd.; the stabilities of the fullerenes are discussed on the basis of the results. The trend in the stabilities predicted by the TRE model is compared with predictions from the conjugated-circuit model as well as the MNDO and ab-initio methods. Reasonable agreement was found between the TRE model and rigorous quantum-mech. methods.

IT 144161-03-5, [5,6]Fullerene-C36-D6h
(topol. resonance energy and Kekule structures of, matching-polynomial algorithms in calcns. of)

L27 ANSWER 16 OF 21 HCPLUS COPYRIGHT 2001 ACS

1994:200593 Document No. 120:200593 Exhaustive Generation and Analytical Expressions of Matching Polynomials of Fullerenes C₂₀-C₅₀. Balasubramanian, K. (Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ, 85287-1604, USA). J. Chem. Inf. Comput. Sci., 34(2), 421-7 (English) 1994. CODEN: JCISD8. ISSN: 0095-2338.

AB The authors consider exhaustive generation of matching polynomials of all fullerenes C_n (n = 20-50, for all even n except C₂₂). Matching polynomials thus computed provide a basis for the derivation of an exact anal. formula for the 1st 8 coeffs. of the matching polynomials of fullerenes. Only the ninth coeff. of the matching polynomial can discriminate structural differences of 2 isomers of fullerenes.

IT 144161-03-5, Fullerene-C36-D6h
(exhaustive generation and anal. expressions of matching polynomials of)

L27 ANSWER 17 OF 21 HCPLUS COPYRIGHT 2001 ACS

1993:656879 Document No. 119:256879 Spectral moments of fullerene cages. Zhang, Hongxing; Balasubramanian, K. (Dep. Chem. Biochem.,

Arizona State Univ., Tempe, AZ, 85287-1604, USA). Mol. Phys., 79(4), 727-45 (English) 1993. CODEN: MOPHAM. ISSN: 0026-8976.

AB Based on the sym. method, anal. expression or recursive relations for the spectral moments of the C₂₀, C₂₄, C₂₆, C₂₈, C₃₀, C₃₂, C₃₆, C₃₈, C₄₀, C₄₂, C₄₄, C₅₀ and C₆₀ fullerene cage clusters are obtained by factoring the original graphs and the corresponding characteristic polynomials into their smaller subgraphs and subpolynomials. The authors also give numerical results for the spectral moments. It is demonstrated that the sym. method is feasible in enumerating the moments as well as factoring the characteristic polynomials for fullerene cages.

IT 144161-03-5, [5,6] Fullerene-C₃₆-D_{6h}
(spectral moments of)

L27 ANSWER 18 OF 21 HCPLUS COPYRIGHT 2001 ACS
1993:434659 Document No. 119:34659 Enumeration of chiral and positional isomers of substituted fullerene cages (C₂₀-C₇₀). Balasubramanian, K. (Dep. Chem. Biochem., Arizona State Univ., Tempe, AZ, 85287-1604, USA). J. Phys. Chem., 97(27), 6990-8 (English) 1993. CODEN: JPCHAX. ISSN: 0022-3654.

AB Enumeration of chiral isomers of substituted fullerene cages (C₂₀-C₇₀) is considered using the generalized character cycle index (GCCI) of the alternating representation of the point group of the parent cage. There are no chiral isomers for the monosubstituted C₂₀, C₂₄, C₂₈, C₃₀, C₃₆, and C₆₀ fullerene cages but there are chiral isomers for other monosubstituted cages. All cages considered here possess chiral isomers for disubstituted cages. The no. of positional isomers can be obtained using the GCCI of the totally sym. representation.

IT 144161-03-5D, [5,6] Fullerene-C₃₆-D_{6h}, hydrogenated
(chiral and positional isomers of, enumeration of)

L27 ANSWER 19 OF 21 HCPLUS COPYRIGHT 2001 ACS
1993:132538 Document No. 118:132538 Enumeration of isomers of substituted C₂₀-C₅₀ fullerene cages. Balasubramanian, K. (Dep. Chem. Biochem., Arizona State Univ., Tempe, AZ, 85287-1604, USA). Chem. Phys. Lett., 202(5), 399-405 (English) 1993. CODEN: CHPLBC. ISSN: 0009-2614.

AB Computerized enumerative combinatorial techniques, which employed quadruple precision arithmetic, were used to enumerate the isomers of hydrogen and fluorine polysubstituted C₂₀-C₅₀ fullerene cages.

IT 144161-03-5D, [5,6] Fullerene-C₃₆-D_{6h}, hydrogenated
(enumeration of isomers of)

L27 ANSWER 20 OF 21 HCPLUS COPYRIGHT 2001 ACS
1993:110079 Document No. 118:110079 Matching polynomials of fullerene clusters. Balasubramanian, K. (Dep. Chem. Biochem., Arizona State Univ., Tempe, AZ, 85287-1604, USA). Chem. Phys. Lett., 201(1-4), 306-14 (English) 1993. CODEN: CHPLBC. ISSN: 0009-2614.

AB Matching polynomials of graphs for fullerene cages for C₂₀-C₅₀ were calcd. and analyzed. Based on these results, the first few coeffs.

of the matching polynomials of C60-C90 cages were obtained. The matching polynomials thus computed are useful in the characterization of aromaticities, computation of the grand canonical partition functions, resonance energies, thermodyn. properties, topol. indexes, and properties of these cages.

IT 144161-03-5, [5,6]Fullerene-C36-D6h
(matching polynomials for)

L27 ANSWER 21 OF 21 HCAPLUS COPYRIGHT 2001 ACS
1992:497761 Document No. 117:97761 Relative stabilities of fullerene, cumulene, and polyacetylene carbon structures for C_n, n = 18-60. Feyereisen, Martin; Gutowski, Maciej; Simons, Jack; Almlöf, Jan (Chem. Dep., Univ. Utah, Salt Lake City, UT, 84112, USA). J. Chem. Phys., 96(4), 2926-32 (English) 1992. CODEN: JCPSA6. ISSN: 0021-9606.

AB The relative stabilities of closed fullerene, cumulene, and polyacetylene carbon structures, as well as the cohesive energies for clusters of size n = 18, 20, 22, 24, 26, 28, 30, 32, 34, 36, 50, and 60 have been examd. using ab initio self-consistent-field and second-order Moeller-Plesset perturbation theory and anal. deriv. geometry optimization methods. These geometries and relative stabilities constitute the primary findings of this work. All calcns. were carried out using the DISCO program with at. basis sets derived from van Duijneveldt's carbon (6s,3p) primitive orbital basis set, contracted to [3s2p]. For n > 32, the fullerenes are predicted to be the most stable, and their cohesive energies are predicted to increase monotonically as n varies from 24 to 60. The optimized geometries obtained here are very near those obtained earlier by others for the few species where such data exist. Based on earlier work employing larger AO bases, the relative energies of the fullerene structures are expected to be lowered even further as larger basis sets are employed. Hence, it is likely that the smallest cluster for which the fullerene structure is the most stable has n < 32. Comparing the computed electron binding energy for C24- to the exptl. vertical detachment energy of this species supports the claim that n = 24 may be the smallest energetically favored fullerene.

IT 144161-03-5, [5,6]Fullerene-C36-D6h
(structure and stability of, ab initio calcn. of)

=> d 131 1-11 ti

L31 ANSWER 1 OF 11 HCAPLUS COPYRIGHT 2001 ACS
TI Structure and stability of solid C36

L31 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2001 ACS
TI Theoretical study for exohydrogenates of small fullerenes C28.appx.C40

L31 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2001 ACS

TI Computing less-rounded cages: C36 non-IPR fullerenes and quasi-fullerenes

L31 ANSWER 4 OF 11 HCPLUS COPYRIGHT 2001 ACS
TI Solid C36: Crystal structures, formation, and effects of doping

L31 ANSWER 5 OF 11 HCPLUS COPYRIGHT 2001 ACS
TI Weighted HOMO-LUMO energy separation as an index of kinetic stability for fullerenes

L31 ANSWER 6 OF 11 HCPLUS COPYRIGHT 2001 ACS
TI D6h C36 molecular dynamics simulations

L31 ANSWER 7 OF 11 HCPLUS COPYRIGHT 2001 ACS
TI Sample applications of an algorithm for the calculation of the number of isomers with more than one type of achiral substituent

L31 ANSWER 8 OF 11 HCPLUS COPYRIGHT 2001 ACS
TI Computational studies on C36 and its dimer

L31 ANSWER 9 OF 11 HCPLUS COPYRIGHT 2001 ACS
TI C36, a hexavalent building block for fullerene compounds and solids

L31 ANSWER 10 OF 11 HCPLUS COPYRIGHT 2001 ACS
TI Molecular structure and dynamical properties of C36: a semi-empirical calculation

L31 ANSWER 11 OF 11 HCPLUS COPYRIGHT 2001 ACS
TI Scanning tunneling spectroscopy of C36

=> d 131 1,4,8,9,10 cbib abs hitrn

L31 ANSWER 1 OF 11 HCPLUS COPYRIGHT 2001 ACS
1999:730383 Document No. 132:142216 Structure and stability of solid C36. Menon, Madhu; Richter, Ernst (Department of Physics and Astronomy, University of Kentucky, Lexington, KY, 40506-0055, USA). Phys. Rev. B: Condens. Matter Mater. Phys., 60(19), 13322-13324 (English) 1999. CODEN: PRBMDO. ISSN: 0163-1829.
Publisher: American Physical Society.

AB Structure and stability of synthesized C36 solid [C. Piskoti et al. (1998)] was investigated using a generalized tight-binding mol.-dynamics method. Out of the many solid forms considered, the most stable structure consists of a polymeric phase of C36 with mixed sp₂ and sp₃ bonding for the atoms. The crosslinking is found to be across the hexagonal faces with strong covalent intermol. coupling. Furthermore, formation of this polymer is found to be an exothermic process. The structural properties are consistent with expt.

IT 144161-03-5, [5,6]Fullerene-C36-D6h
(structure and stability of solid C36 studied by generalized

tight-binding mol.-dynamics method)

L31 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2001 ACS
 1999:576496 Document No. 131:330136 Solid C36: Crystal structures, formation, and effects of doping. Grossman, Jeffrey C.; Louie, Steven G.; Cohen, Marvin L. (Materials Sciences Division, Department of Physics, Lawrence Berkeley National Laboratory, University of California at Berkeley, Berkeley, CA, 94720, USA). Phys. Rev. B: Condens. Matter Mater. Phys., 60(10), R6941-R6944 (English) 1999. CODEN: PRBMDO. ISSN: 0163-1829. Publisher: American Physical Society.

AB The authors employ plane-wave pseudopotential d. functional calcns. to show that the lowest energy D6h C36 crystal is a highly bonded network of hexagonal planes of C36 units with AB stacking. This crystal is significantly more dense and lower in energy than previously proposed structures. Na is the largest alkali atom that can be intercalated into the crystal structure without causing severe structural distortion. Further, the authors predict the reaction pathway to form a neutral C36 dimer to be barrierless, while neg. charged C36 mols. are less likely to bond due to a substantial barrier of formation.

IT 144161-03-5, [5,6]Fullerene-C36-D6h
 (solid C36: crystal structures, formation, and effects of doping)

L31 ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2001 ACS
 1999:326447 Document No. 131:107063 Computational studies on C36 and its dimer. Jagadeesh, Mavinahalli N.; Chandrasekhar, Jayaraman (Department of Organic Chemistry, Indian Institute of Science, Bangalore, 560 012, India). Chem. Phys. Lett., 305(3,4), 298-302 (English) 1999. CODEN: CHPLBC. ISSN: 0009-2614. Publisher: Elsevier Science B.V..

AB The energetics of three competing low-energy isomers of C36 (D6h, D2d and C2v forms) in their singlet and triplet states were computed at the AM1, HF/3-21G, HF/6-31G* and B3LYP/6-31G* levels. The most stable structure is predicted to be the D6h isomer with a triplet ground state of 3A2u symmetry. This electronic structure can account for the 'covalent' interactions noted in solid C36. The dimeric structure with D2h symmetry was optimized using the AM1 and HF/3-21G methods. Dimerization is calcd. to be energetically favorable. Important changes expected due to dimerization in the vibrational and electronic spectra are pointed out.

IT 144161-03-5, Fullerene C36 D6h
 (computational studies on C36 and dimer)

L31 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2001 ACS
 1999:58284 Document No. 130:257556 C36, a hexavalent building block for fullerene compounds and solids. Fowler, P. W.; Heine, T.; Rogers, K. M.; Sandall, J. P. B.; Seifert, G.; Zerbetto, F. (School of Chemistry, University of Exeter, Exeter, EX4 4QD, UK). Chem. Phys. Lett., 300(3,4), 369-378 (English) 1999. CODEN: CHPLBC. ISSN: 0009-2614. Publisher: Elsevier Science B.V..

AB Structures and energies were calcd. at the DFTB level for C36-based

fullerenes, hydrides, oligomers and solids. The two fullerenes with minimal pentagon adjacencies are isoenergetic. The isomer implicated in recent expts. has C6v broken symmetry, a small HOMO-LUMO gap and can gain or lose up to six electrons. C36 forms stronger inter-cage bonds than larger fullerenes. A favored sigma.-bonding pattern rationalizes a dimer with ten times the stabilization of (C60)2, a linear polymer, a 'superbenzene' oligomer, a 'supergraphite' layer and a hcp. solid with a monomer stabilization of 522 kJ mol-1 and a d-spacing (6.82 Å) compatible with the expts.

IT 144161-03-5, [5,6]Fullerene-C36-D6h

(tight-binding DFT study of C36 as hexavalent building block for fullerene compds., superbenzene, supergraphite layer, and solids)

L31 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2001 ACS

1999:44551 Document No. 130:158675 Molecular structure and dynamical properties of C36: a semi-empirical calculation. Halac, E.; Burgos, E.; Bonadeo, H. (Departamento de Fisica, Comision Nacional de Energia Atomica, San Martin, Pcia. de Buenos Aires, 1650, Argent.). Chem. Phys. Lett., 299(1), 64-68 (English) 1999. CODEN: CHPLBC. ISSN: 0009-2614. Publisher: Elsevier Science B.V..

AB We have explored possible mol. structures and calcd. the vibrational properties of the newly synthesized C36 fullerene. We used a semi-empirical covalent potential that has been shown to reproduce these properties well in C60, C70, diamond and graphite. In agreement with ab initio calcns., we find that D6h and D2d structures are the most stable. Using our semi-empirical potential we obtain IR frequencies in the range of those obsd. for the crystal powder. We also calc. the Raman spectrum on the basis of the band polarizability model.

IT 144161-03-5, Fullerene (C36) D6h

(semi-empirical calcn. of mol. structure and dynamical properties of C36)

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(FILE 'HCAPLUS' ENTERED AT 15:22:28 ON 31 JUL 2001)

FILE 'REGISTRY' ENTERED AT 15:34:25 ON 31 JUL 2001

FILE 'HCAPLUS' ENTERED AT 15:34:33 ON 31 JUL 2001

FILE 'REGISTRY' ENTERED AT 15:50:34 ON 31 JUL 2001

FILE 'HCAPLUS' ENTERED AT 15:50:42 ON 31 JUL 2001

L32 54 S L13 NOT (L4 OR L5 OR L6 OR L7 OR L8 OR L9)

L33 21 S L32 AND 1967-1998/PY

L34 0 S L33 NOT (L26 OR L27 OR L31)

L35 33 S L32 AND 1967-1999/PY

L36 0 S L35 NOT (L26 OR L27 OR L31)